Enhancing Hit Identification in *Mycobacterium tuberculosis* Drug Discovery Using Dual-Event Bayesian Models

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Running Head: Dual Event Bayesian Models

Figure S6. TB kinase dose response model: bad features from FCFP_6.

NH NH	O N	NH O SS O	NH S *	NH *
B1: 1183237506	B2: 984117435	B3: -1482227438	B4: 1176920513	B5: 1980808403
0 out of 9 good	0 out of 8 good	0 out of 8 good	0 out of 7 good	0 out of 7 good
Bayesian Score: -1.747	Bayesian Score: -1.650	Bayesian Score: -1.650	Bayesian Score: -1.544	Bayesian Score: -1.544
NH S	NH NH	NH ₂ ONH NH _S NH	* NH NH *	» NH *
B6: 1122517666	B7: 1474973492	B8: -532506075	B9: -551147930	B10: 469153063
0 out of 7 good	0 out of 7 good	0 out of 6 good	0 out of 6 good	0 out of 6 good
Bayesian Score: -1.544	Bayesian Score: -1.544	Bayesian Score: -1.425	Bayesian Score: -1.425	Bayesian Score: -1.425

S N	N *	S ₊	» NH	Z=0
B11: -470831435	B12: -446103674	B13: 633795852	B14: 1415816015	B15: 1786546801
0 out of 6 good				
Bayesian Score: -1.425				
NH ₂	NH O I O I		O * * * * *	* N * *
B16: 471397705	B17: -863010654	B18: -720826636	B19: 1867039149	B20: 1889594586
0 out of 6 good	0 out of 6 good	0 out of 6 good	1 out of 12 good	0 out of 5 good
Bayesian Score: -1.425	Bayesian Score: -1.425	Bayesian Score: -1.425	Bayesian Score: -1.297	Bayesian Score: -1.289